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Simulations of equilibrium magnetic and magnetoelastic properties of non-conducting rare-earth compounds

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Abstract

© Kazan Federal University (KFU).The Hamiltonian of the magnetic subsystem containing rare-earth ions involves energies of the localized 4f-electrons in free ions, energies of interactions of the 4f-electrons with the static crystal field in the perfect crystal lattice as well as in the homogeneously deformed lattice, interactions with the external magnetic field and lattice vibrations (electron-phonon interaction), magnetic dipolar and exchange interactions between the ions. This Hamiltonian is used in calculations of different measurable physical parameters versus temperature and the magnetic field strength and direction (energy levels of rare earth ions, the magnetization, magnetic dc- and ac-susceptibilities, elastic constants, lattice deformations).

Keywords

Crystalline electric field parameters, Electron-phonon interaction, Magnetoelastic interaction, Magnetostriction